Atomistic simulation of adsorbed water layer in nanoporous silica: implications on oil recovery

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Recently, the physicochemical properties of fluids confined in nanoporous rocks have been attracting considerable attention. For water-oil-rock interfaces, it is expected to have a water layer between the mineral surface and the confined oil. Properties like, interfacial tension and injection pressure could be affected by the presence of this water layer and the understanding of their behavior under confined conditions are needed to improve oil recovery. Here, we have performed non-equilibrium molecular dynamics (NEMD) of fluid (H_2O and oil) flow inside amorphous silica cylindrical nanopores. The structural and thermodynamical properties of the fluids inside the pores were studied. The crude oil was modelled as a combination of alkanes, cycloalkanes and aromatic hydrocarbons. An oil flux was induced on an initially water-filled pore (4 nm). A water layer of about 6 Å thick is observed between the silica surface and the oil phase (Fig.1). By atomistic simulations, we could determine: i) the critical pressure necessary to have the oil penetrating in nanoporous (~1000 atm), ii) the presence of the water layer alters the interfacial tension by an order of magnitude, and iii) the molecular ordering. The results of confined crude oil differ significantly from the one with a water layer adsorbed on the nanoporous surface.

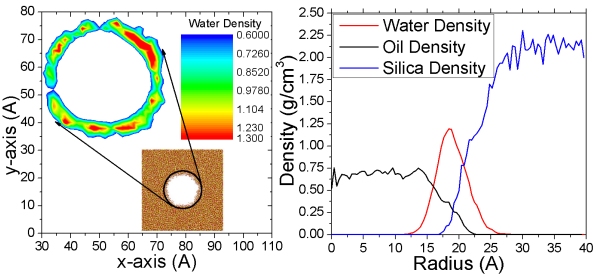

Figure 1: Density map of the water layer confined in the nanopores (left). Densities of water, oil and silica, within the 4 nm nanopore (right).